MM 25: Development of Computational Methods: Crystal Structure and Properties

Time: Wednesday 10:15–11:30   Location: SCH A 251

MM 25.1   Wed 10:15   SCH A 251

A hybrid multiscale phase-field crystal, amplitude phase-field crystal approach - elastic properties and numerical studies — •MAIK PUNKE and MARCO SALVALAGLIO — Technische Universität Dresden, Institut für Wissenschaftliches Rechnen, Bürogebäude Z21, Zellescher Weg 25, 01217 Dresden

The modeling of crystalline materials requires the resolution of microscopic details on large length and time scales to guarantee the description of lattice-dependent features as well as the dynamics of solidification. The so-called phase-field crystal (PFC) model emerged as a prominent framework to model crystalline systems. Indeed, it describes crystalline materials through a continuous order parameter related to the atomic number density and its dynamic at relatively large (diffusive) time scales. The amplitude expansion of the PFC model (APFC) was developed to further overcome the length scale limitations in the PFC framework. Herein, the continuous density in PFC models is replaced by the amplitudes of the minimum set of Fourier modes (wave vectors) for a given crystal symmetry.

We propose a multiscale model with local PFC accuracy and APFC length scale limitations. In our hybrid multiscale approach, the PFC and APFC models are coupled through Dirichlet conditions by penalty terms within the spectral framework. We showcase the model capabilities via selected numerical investigations which focus on the energetic and elastic properties of two-dimensional crystals. Furthermore, runtime and accuracy comparisons with the standard PFC and APFC models are made.

MM 25.2   Wed 10:30   SCH A 251

Corrosion evolution in Mg-based alloys: the role of precipitates studied by synchrotron X-ray nanotomography — •TATIANA AKHMETSHINA[1], ROBIN E. SCHÄUBLIN[1], ANDREA M. RICH[1], NICHOLAS W. PHILLIPS[2], and JÖRG F. LÖFFLER[1] — [1]Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, Switzerland — [2]Paul Scherrer Institute, 5232 Villigen PSI, Switzerland

Magnesium alloys are very promising candidates for light-weight and bioresorbable medical applications. However, being an active metal, magnesium is susceptible to localized corrosion caused by precipitates or solute elements. In this work, we compare the corrosion behaviour of lean Mg-Ca (X0), developed in our laboratory, with the well-known Mg-Y-Nd-Zr (WE43) alloy that is currently deployed as biomedical material. X0 alloys (0.2-0.6 wt.% Ca) offer a combination of high strength and high ductility and can be considered a safe substitute for WE43 in bioresorbable implants. Using the 3D ptychography technique at the cSAXS beamline of the Swiss Light Source, we monitored the corrosion evolution in X0 and WE43. Both exhibit very different precipitates, which can be distinguished by their electron density in X-ray imaging. We found that the rare-earth-rich precipitates in WE43 tend to remain in the corrosion layer, whereas the Ca-rich ones in X0 predominantly dissolve without any pitting effect. The appearance of the corrosion product and the related chemical composition were also quite different. These findings of in-vitro corrosion can help to better understand the in-vivo degradation of Mg-based biomedical devices.

MM 25.3   Wed 10:45   SCH A 251

Amplitude expansion of the phase-field crystal model for complex crystal structures — •MARCELLO DE DONNO[1] and MARCO SALVALAGLIO[1,2] — [1]Institute of Scientific Computing, Technische Universität Dresden, 01062 Dresden, Germany — [2]Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden, Germany

The phase field crystal model allows for studying phenomena on atomic length and diffusive time scales. It accounts for elastic and plastic deformation in crystals, including several processes such as crystal growth, dislocation dynamics, and microstructure evolution. The amplitude expansion of the phase field crystal model describes the atomic density by a small set of slowly-oscillating Fourier modes, making it possible to tackle large three-dimensional systems. However, only basic crystal symmetries have been studied so far. We present a general treatment of virtually any lattice symmetry using the amplitude phase field crystal model, incorporating approaches originally proposed for the phase field crystal model which enable the treatment of non-trivial lattices. We discuss the stability of selected crystal structures, focusing on non-Bravais lattices. As pivotal examples, we show that the proposed approach allows a coarse-grained description of the kagome lattice, exotic square arrangements, and the diamond lattice, hosting dislocations.

MM 25.4   Wed 11:00   SCH A 251

Efficient molecular dynamics simulations using fourth-generation neural network potentials — •EMIR KOCER[1,2], ANDREAS SINGRABER[3], TSZ WAI KO[1,2], JONAS FINKLER[4], PHILIPP MISOF[3], CHRISTOPH DELLAGO[3], and JÖRG BEHLER[1,2] — [1]Lehrstuhl für Theoretische Chemie II, Ruhr-Universität Bochum, Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Bochum, Germany — [3]Institut für Experimentalphysik, Universität Wien, Wien, Austria — [4]Departement Physik, Universität Basel, Basel, Switzerland

Machine learning potentials (MLP) have become a common tool in materials modelling due to their ability to bridge the gap between ab initio and classical molecular dynamics. A limitation of most MLPs, however, is the locality approximation in that only interactions within a cutoff range are considered. This could lead to inaccurate dynamics in systems with relevant long-range interactions. Recently, a fourth-generation of MLPs has emerged that can take also global phenomena like non-local charge transfer into account. An example is the fourth-generation high-dimensional neural network potential (4G-HDNNP), which utilizes a global charge equilibration. In this study, a modified version of 4G-HDNNPs with enhanced efficiency will be presented. The new algorithm has been implemented in the LAMMPS software and tested in large-scale molecular dynamics simulations.

MM 25.5   Wed 11:15   SCH A 251

Sampling-free determination of accurate free energies: A bond lattice mean-field model for central potentials — •RAYNOL DSOUZA[1], THOMAS SWINBURNE[2], LIAM HUBER[3], and JÖRG NEUGEBAUER[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — [2]CINaM, Campus de Luminy, 13288 Marseille, France — [3]Grey Haven Solutions, Victoria, Canada

The computation of accurate anharmonic free energies at finite temperatures commonly involves the sampling of a large number of configurations. The commonly used (quasi)-harmonic approximation sacrifices physical fidelity by only sampling very few of these configurations. A recent study by the co-authors showed that a mean-field of a lattice of uncorrelated anharmonic first nearest-neighbour bonds can be used to approximate anharmonic free energies of fcc crystals with meV/atom accuracy when paired with a polarized bonding potential [1], thus recapturing an approximation of the anharmonic contributions with minimal computational expense. We extend this approach to central potentials, while maintaining the original constraints of material compatibility and thermodynamic self-consistency of the model. Using a parameterized bonding potential generated from a few T=0 K ab initio calculations [2] for fcc aluminium, we show that the model yields free energies close to meV/atom of those calculated from ab initio thermodynamic integration for a fraction of the computational effort. [1] Swinburne et al., Phys. Rev. B 102, 100101(R) (2020) [2] Glensk et al., Phys. Rev. Lett. 114, 195901 (2015)